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Closing the gap: Exploring the limits of lubrication theory via molecular dynamics AMIR M. RAHMANI, MEHLAM JUPITERWALA, YANG SHAO, CARLOS E. COLOSQUI, Department of Mechanical Engineering, Stony Brook University — Advances in nanofabrication allow the engineering of nanoelectromechanical systems and nanofluidic devices with dimensions on the order of 1 to 100 nanometers. Lubrication flows with characteristic lengths approaching the molecular scale have become ubiquitous in a wide spectrum of applications ranging from biomass sensing and atomic force microscopy to drug delivery and synthesis of nanomaterials. At nanometer scales, the effects of thermal fluctuations, disjoining pressure, and finite atomic size produce various phenomena beyond the reach of classical continuum hydrodynamics. We will present a theoretical and computational study on nanoscale lubrication flows where bodies immersed in dense fluid media either are kept under static conditions or are allowed to undergo thermal fluctuations about a prescribed position. We find that under static conditions, continuum-based lubrication models can accurately predict hydrodynamic forces computed via molecular dynamics simulations at surprisingly small scales (i.e., for flows having subnanometer-sized lubrication gaps). Thermal vibration, however, can induce drag reduction and other dynamic effects that can potentially be described by extending conventional lubrication models.

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